Accelerated Strategic Computing Initiative

ASCI at Livermore

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LLNL and LANL Meet FY2001 V&V Level-1 Milestone

The ASCI Verification and Validation (V&V) Program, officially launched in FY1999, reports that LLNL and LANL achieved the FY2001 Q2 Level-1 Milestone for the "Demonstration of an Initial Validation Methodology for the Current State of ASCI Code Modeling for Early-Time Primary Behavior." An independent panel must certify the achievement of this level-1 milestone in a July 2001 review.

The ASCI V&V Program is responsible for independent evaluation of the quality of the code development products for ASCI-level simulation capability. This "Initial Validation Methodology" milestone is the first of a series of V&V level-1 milestones planned through FY2005.

The milestone exercised the current validation methodology on ASCI codes for the simulation of the performance of stockpile primary devices in their early hydrodynamic phase, before the production of nuclear energy. The methodology was demonstrated with 3D simulations performed on ASCI codes. The purpose of the milestone was to demonstrate the methodology for the application area of primary hydrodynamic performance, rather than to validate the actual code capability.

A full-length article covering the achievement of this V&V level-1 milestone will be published in a future edition of *ASCI at Livermore*.

Crandall Dedicates LLNL's Visualization Work Center

On March 21 (LLNL's Science Day), David Crandall, Assistant Deputy Administrator for Research Development and Simulation at DOE, dedicated the latest of ASCI's achievements at LLNL—The ASCI Visualization Work Center in Building 111.

The Laboratory's Visualization Work Center is designed to help Defense and Nuclear Technology scientists visualize the results of their computer simulations and compare them to experimental results. Advanced computational simulations coupled with 3D modeling are considered vital components of DOE's Stockpile Stewardship Program. Visualization for ASCI-sized problems necessitates a comprehensive solution based on state-of-the-art hardware, leading-edge visualization research, and a synthesis of commercial tools with in-house software.

According to Steve Langer, who coordinates visualization activities for A-Program, "ASCI needs visualization centers to deal with the enormous volume of data generated by a 3D simulation. One of my colleagues ran a simulation of an ICF capsule that created 1.5 terabytes (1500 gigabytes) of disk files describing what happened during the simulation. There have been quite a few runs on the ASCI computers that have generated file sets even larger

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From the left, A-Program's Steve Langer helps David Crandall cut the ribbon at the dedication of the Visualization Work Center in Building 111. David Nowak (right) notes the use of ASCI-sized scissors.

than that, and they will only become larger in the future.

"It is impossible to look at any significant fraction of those numbers without using graphics. The human brain is designed to look at images and discover features (such as lines, color changes, patterns obscured by irrelevant detail, etc.) very rapidly. We are relying on that capability to let code developers find errors in simulations and to let designers assess the quality of a simulation. A bad line of code can lead to an erroneous temperature, for example, in a few zones that then spreads throughout the problem and invalidates the results. By sweeping a slicing plane (the plane is false-colored based on temperature) through the simulation, it is often easy to spot the zones with the problem. Scrolling through a table of a few million numbers in a text editor doesn't work.

"Graphical analysis has a similar advantage for a designer who is running a simulation of interest to Stockpile Stewardship. The designer has to decide whether he or she had fine enough spatial resolution and whether all the important physical processes were modeled. We are still in the early stages of figuring out which visualizations are most helpful for designers, but I have already made a few visualizations that revealed something unexpected about a simulation."

Visualization Work Center Layout

The Visualization Work Center is designed to function for small group interactions and for presentations to larger groups. It can display results using several different display technologies and has room to test new technologies, as they become available. The largest display in the Visualization Work Center is the Power Wall, which is driven by eight projectors. The projectors are arranged in a 4 × 2 array behind the screen and are aligned to generate a single 5120- × 2048-pixel image. The 4 × 2 screen will often be split into two 2 × 2 sections to provide easy side-by-side comparison of two simulations. This room has another screen driven by a single projector that can be connected to a VCR or to a laptop computer. This screen is normally used to display slides from an application such as PowerPoint while leaving the Power Wall free to display simulations. The room can seat up to three dozen people when used as a theater, but the chairs can be moved aside to provide an open space in which smaller groups can explore and discuss their visualizations.

There are two smaller rooms in the Visualization Work Center. One room currently has a 1920- × 1200-pixel CRT screen, which is the same as those installed in ten offices in Building 111. This CRT provides access to visualization capabilities for those who do not have them in their own offices. Future possibilities for this room include installing a projector that can display stereo images for viewing by small groups and housing one of the extremely high-resolution LCD panels, which are just emerging from research laboratories.

The second small room also has a 1920- × 1200-pixel CRT. Its distinctive feature is a "personal Power Wall," which is made up of four 1280- × 1024-pixel LCD panels arranged in a 2 × 2 grid. This display allows a scientist to examine a simulation at higher resolution than is possible in an office.

An SGI visualization engine called *Edgewater* drives the displays in the Visualization Work Center. Edgewater is located in another building at LLNL and connected to the Visualization Work Center by means of fiber optic modems. Edgewater provides the computational power and high disk transfer rates needed to rapidly generate visualizations from large 3D data sets.

This new Visualization Work Center met its customer's first deadline. The Power Wall and Presentation Screen capabilities were fully operational in time for use with the ASCI Level-1 Milestone Review on January 17 and 18, 2001.

VIEWS Acknowledgments

Steve Langer is quick to acknowledge the efforts of Bob Howe, LLNL VIEWS Operations Project Lead. "Bob arranged for the Plant Operations people to actually construct the Visualization Work Center, he supervised the procurement process, and he was our main contact for design." In addition to Langer and Howe, the managers and principal contributors to this Visualization Work Center effort are listed below:

VIEWS Program Manager, NNSA HQ: John van Rosendale

LLNL ASCI Management:
David Nowak and Randy Christensen

LLNL DNT Management:
Charlie Verdon, Richard Ward, Jim Rathkopf, and Doug Post (LANL)

LLNL SCCD Management:
Mike McCoy, Steve Louis, and Terri Quinn

LLNL Plant Engineering Lead for this project: Mike Atkinson

LLNL VIEWS Visualization Project Lead: Randy Frank

Design review:
Joyce Moulden and Ellen Tarwater

Design and construction:
Ike Fernandez, Earle Glenn, and Asya Mandelbaum

LLNL VIEWS Project Members—SGI computer systems:
Michael Atzet, Rich Fischer, and Dale Southard

LLNL VIEWS Project Members—projectors and integration:
Ross Gaunt and Scott Miller

LLNL VIEWS Project Member—SGI resource management:
Peter Norquist

Networking and fiber deployment:
Jay Drew, Steve Hoit, Lynn Jepson, and Joe Slavec

Security plans: Robert Justice, Candy Nelson, Gina Pepper, Kim Silva, Dave Wiltzius, and Bing Young

Administrative support:
Melissa Odom

LLNL's Science Day Features Terascale Computing

On March 21, Science Day focused on scientific supercomputing and how LLNL can meet the next decade of national challenges through the integration of theory, experiments, technology, and large-scale simulation. The Laboratory's Science Day presentations also showed how ASCI terascale computing plays a significant role in research conducted over a cross-section of Laboratory directorates and programs.

Bill Dannevik, the Deputy Associate Director for Science and Technology in the Energy and Environment Directorate, discussed how terascale simulation is a powerful tool for numerical exploration of the behavior of strongly turbulent flow. Dannevik and his team earned the coveted *Gordon Bell Prize* for their work in 1999.

Tomas Diaz De La Rubia, the Materials Program Leader for NIF, addressed how the advent of large, massively parallel computers capable of doing trillions of operations per second has advanced research into predicting the properties and performance of materials from fundamental physical principles.

Jave Kane, a postdoctoral research associate at the Institute for Laser Science and Applications in the University Relations Program, showed how lasers are being used to recreate some astrophysical phenomena in the laboratory. In his survey called "Scaling Astrophysics into the Laboratory," Jave used Grant Bazan's published ASCI code calculations of 3D supernova hydrodynamic instabilities.

David Cooper, Associate Director for the Computation Directorate and Chief Information Officer, discussed the role of high-performance simulation capabilities in the Stockpile Stewardship Program. He summarized the current terascale computing environment plus future strategies and industrial partnerships.

Giulia Galli, the Quantum Simulation Group Leader from the Physics and Advanced Technologies Directorate, showed recent results obtained at LLNL using quantum molecular dynamics. She illustrated state-of-the-art investigations of both physical and chemical properties of condensed matter systems and analyzed the key role of quantum simulations in the study of complex systems.

Michael Colvin, a team leader in the Computational Biology Group, discussed the expanding role of computational simulations in biological research. He reviewed several computational methods for biological simulation and described the application of the methods.

Starley Thompson, a scientist from the Climate and Carbon Cycle Modeling Group in the Energy and Environment Directorate, surveyed three areas of current LLNL computational climate science: (1) Ocean Carbon Sequestration, (2) Integrated Climate and Carbon Simulation, and (3) High-resolution Global Atmospheric Simulation.

David McCallen, Director of the Center for Complex Distributed Systems in the Engineering Directorate, noted that "Emerging high-performance computer capabilities offer the potential for realistic simulations of complex earthquake processes." He presented results of recent LLNL large-scale computer simulations of seismic wave propagation in the Bay Area and the response of the Bay Bridge to potential earthquakes in the future.

For further information on the Science Day presentations and posters, please visit LLNL's Science Day website at http://stars.llnl.gov/ScienceDay/index.html

Dennis Hewett to Represent ASCI at Stanford

Dennis Hewett of X Division has agreed to serve as the LLNL representative on the ASCI Alliance Tri-lab Sponsor Team (TST) for Stanford University's Center for Integrated Turbulence Simulations. The role of the TST is to help form connections between the Alliance Centers and Laboratory scientists who have similar interests and to assist in the success of those Centers. ASCI Program Leader David Nowak notes, "Dennis' extensive interest and background in kinetic and fluid modeling matches well with Stanford's research program. Dennis is also a pilot and has a strong interest in all aspects of aircraft design, including the gas turbines that Stanford is modeling." Dennis replaces Doug Post who transferred to Los Alamos earlier this year.

Dennis Hewett will represent LLNL at ASCI Alliance partner Stanford University.

Dennis Hewett earned his Ph.D. in Plasma Physics from the University of Kansas in 1973. He joined the Laboratory in 1983, following eight years at Los Alamos and two years at MIT. He became a Fellow of the American Physical Society in 1994.

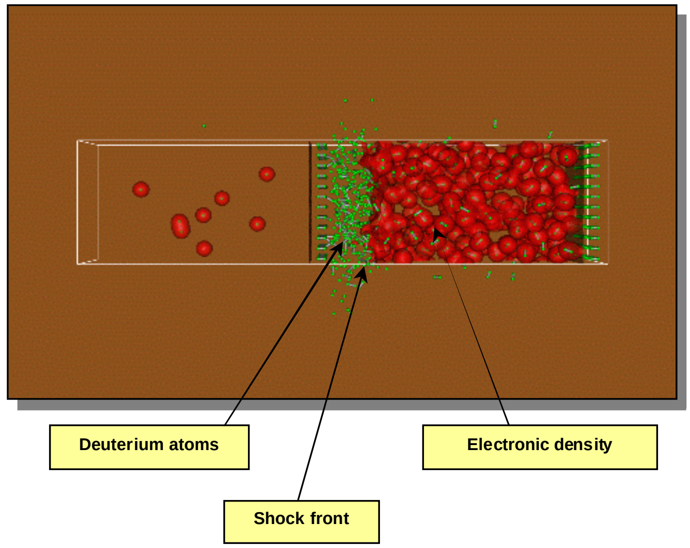
Dennis began flying in 1981 while at Los Alamos and received his instrument rating in 1988 through a flying club in Livermore. Shortly thereafter, he notes that he "adopted" one-third of a 4-passenger Cessna 182, which he happily flies when his schedule permits—and when the other two-thirds are available.

This work was performed under the auspices of the U.S. Department of Energy by University of California Lawrence Livermore National Laboratory under contract No. W-7405-Eng-48.

Large-scale First-Principles Simulations of Shocks in Deuterium

Many researchers have investigated the properties of compressed liquid deuterium over the past decades, using the most advanced theoretical and experimental tools. Recently, new approaches to the exploration of the properties of condensed matter have been made possible through the advent of large-scale high-performance computers, and an increasing number of important contributions to the study of compressed liquids are now coming from numerical simulations. Following the installation of the ASCI White computer at LLNL, we were able to perform for the first time large-scale First-Principles Molecular Dynamics simulations of the formation and propagation of a shock front in liquid deuterium.

First-Principles Molecular Dynamics (FPMD) is a simulation method that incorporates an accurate, quantum mechanical description of atomic-scale interactions. Instead of relying on empirically adjusted models, FPMD depends only on the knowledge of a few fundamental physical constants, and on the atomic identity of the elements composing the system under study. This makes it a method of choice in investigations of condensed matter subjected to extreme conditions—for which experimental data is often scarce—or in regimes where experiments are unfeasible. In particular, FPMD allows no *a priori* assumptions about the formation and disappearance of chemical bonds during a simulation; instead, chemical bonds are allowed to form and break as a consequence of the fundamental laws of physics.



A sample of liquid deuterium subjected to a supersonic impact, showing the formation of a shock front on the atomic scale. The results bring new insight into the interpretation of laser-shock experiments.

This accuracy and versatility are however obtained at the cost of a very large computational complexity. Contrary to conventional molecular dynamics simulations—which now routinely involve millions of atoms—first-principles simulations have been limited to smaller systems, typically including a few hundred atoms. Like many other numerically intensive algorithms, FPMD has greatly benefited from vast increases in available computing power.

The implementation of FPMD developed at LLNL over the past three years was ported to the ASCI White computer in October 2000 and used in early “science runs” on that platform. For the first time, sufficient computational power was available to run first-principles simulations of the propagation of a shock wave in a sample of liquid deuterium. The simulation involved 1320 atoms (see the figure above) and ran for several days on 2640 processors of ASCI White. It provided an extremely detailed picture of the formation and propagation of a shock front on the atomic scale. Atomic trajectories and individual electronic states could be analyzed and followed during the course of the shock propagation, revealing complex mechanisms of molecular dissociation at the shock front.

Such large-scale simulations are necessary in order to confirm or invalidate other models used to describe the equation of state of compressed fluids. Direct confrontation with experiment also provides a test of the accuracy of the quantum mechanical model used in FPMD.

—*Francois Gygi and Giulia Galli*

Next Issue

In the next issue of *ASCI at Livermore*, Jack Reaugh and Stewart Keeton will discuss “High-explosive Simulations in ASCI.”

ASCI at Livermore is published by the Accelerated Strategic Computing Initiative Program, a division of the Defense and Nuclear Technologies Directorate at Lawrence Livermore National Laboratory. Please send corrections and contributions to Tim Peck, (925) 424-6251 and peck7@llnl.gov.